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# computer series, 173

## Bits and Pieces, 53

Guidelines for Authors of Bits and Pieces appeared in July 1986. The number of Bits and Pieces manuscripts is expected to decrease in the future (see the July 1988 and March 1989 issues). Bits and Pieces authors who describe programs will provide listings or machine-readable versions of their programs. Please read each description carefully to determine compatibility with your own computing environment before requesting materials.

### A Self-Paced Computer Tutorial on the Concepts of Symmetry

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Symmetry is a key concept in the physical, chemical, biological, and material sciences. Physicists express many of the most basic relationships of quantum mechanics, nuclear structure, and relativity in terms of symmetry. Electronic orbitals, which determine the chemical properties of atoms and molecules, are classified by symmetry, their most essential characteristic. In biochemistry, many viruses and macromolecules are symmetric, and their symmetry is a property essential to their formation and self-assembly. Chemists and geologists observed long ago that crystals exhibit macroscopic regularity, which led to the basic concept of the unit cell: When repeated periodically in a three-dimensional array, unit cells determine crystal morphology (*1*). From these important ideas, the field of X-ray crystallography was born (*2*), and it remains the single most general experimental method for the determination of molecular structure. Because symmetry serves as a foundation for so many fundamental scientific concepts, it is necessary that chemistry students, as well as students in other scientific disciplines, understand symmetry and be able to visualize rather complex spatial relationships.

Articles in previous issues of *this Journal* (*3*) have addressed the teaching of these concepts. Several studies have indicated that students experience difficulty with many aspects of three-dimensional thinking required for learning and understanding chemistry (*4–9*). Teaching aids—such as models (*10*), diagrams showing successive rotation and reflection (*11*), and two-dimensional projections (*12*)—have been used to ease this difficulty, although students and instructors sometimes find these aids time-consuming and cumbersome. Interactive computer graphics, however, provides a powerful new tool for teaching symmetry. Its flexible, self-paced nature has many advantages over other teaching methods. Transformational aspects of symmetry become more readily apparent with animation.

#### The Animated Interactive Tutorial

To aid students in our physical chemistry courses at California State University, Fullerton to understand better the concepts of symmetry, we have created an animated interactive tutorial using the multimedia capabilities of the Macintosh computer. Simple point-group transformations are applied to familiar objects such as a hand, and to common molecules such as water or benzene. Rules for translation that give rise to two-dimensional lattices are addressed in a module on plane groups. The tutorial can be run as part of a lecture series or made available to students outside of class for self-paced study. The merit of the tutorial, which is described herein, lies not so much in the novelty of the concepts covered, as in the ability of students to readily visualize common symmetry operations.

#### *Hardware and Software Requirements*

The tutorial may be run on a Macintosh II computer or better with at least 5 Mb of memory, and color graphics, preferably with 256 colors. Color is an important distinguishing characteristic of the models used in this program. If viewed on a computer without sufficient color capabilities, the differentiation of objects may be inadequate. Swivel 3D Professional version 1.0 and Macromind Director versions 2.0 and 3.0 have been used to create the images and animate the sequences. The tutorial stands alone with no special applications required to run it on any Macintosh with Hypercard installed. It occupies approximately 3 Mb of memory. Running time is approximately 45 min for a continuous presentation, with each module approximately 2 min in duration.

#### *Features*

To foster an intuitive understanding of symmetry, the objects transformed have been chosen on the bases of familiarity and simplicity. A hand, for example, is used as an asymmetric unit to illustrate the concepts of cyclic, mirror, and dihedral symmetry. Common molecules including water and benzene have been chosen to represent these symmetries. To facilitate the transition from two-dimensional symmetry concepts to three-dimensional ones, two-dimensional symmetry has been shown as imbedded in three-dimensions through the use of perspective.

The tutorial begins with a table of contents, allowing the user to select a desired module. The user can return to this table of contents at any time within the program and step back and forth between modules to review an idea. Each of 20 modules covers a single symmetry group or lattice structure and includes instructions that direct the user through the tutorial. Explanatory or descriptive text appears in highlighted boxes. Throughout the modules both Hermann–Maugin (*13*) and Schoenflies (*14*) point-group notation systems are used in the descriptions.

In the introduction, relevant terms and symbols are defined. The tutorial then progresses through cyclic symmetry, using an image of a hand as the asymmetric unit. As the hands rotate to illustrate the operation that superimposes the system on an image of its original position, a "ghost" of the original image remains on the screen. Mirror symmetry is addressed next, followed by dihedral symmetry (Fig. 1).

The program then moves on to molecular examples of point groups, using the molecules water, ammonia, *t*-1,2-dichloroethene, and benzene to illustrate the point groups $C_{2v}$ (2mm), $C_{3v}$ (3m), $C_{2h}$ (2/m), and $D_{6h}$ (6/mmm). These modules also use a ghost image to demonstrate when the symmetry operations have been completed. Rotation axes and mirror planes fade in and out or slide through the system to depict their "imaginary" nature.

From point groups, the modules continue with rules for translation that give rise to plane groups. The five two-dimensional plane groups for biological systems are covered currently in these modules. A scalene triangle serves as the asymmetric unit here, and the motif is some grouping of triangles (*15*).

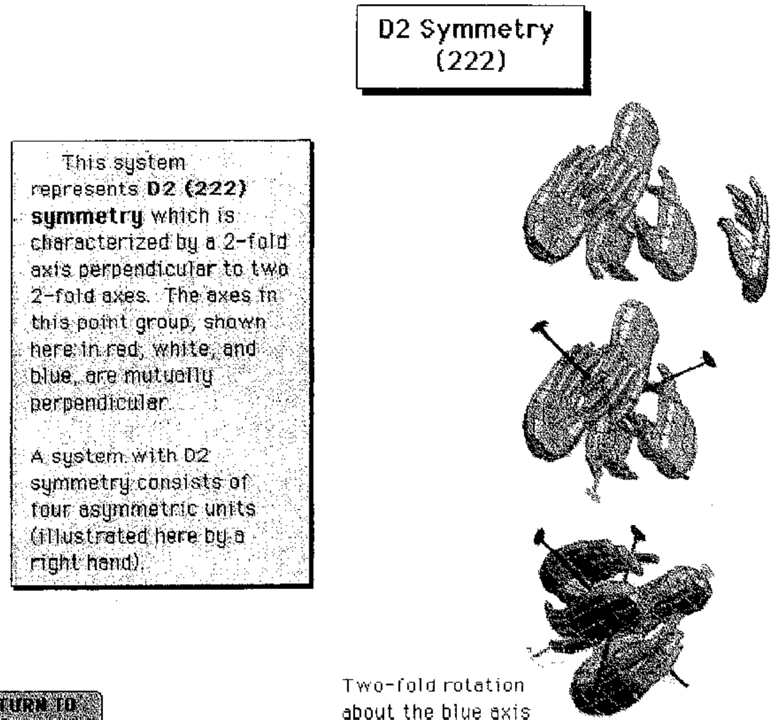


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Figure 1. Dihedral Symmetry. The hand as asymmetric unit is indicated, followed by the principle and 2-fold rotation axes. Rotation about each of the rotation axes is demonstrated. Ghost images of the original positions of the asymmetric units are visible.

## Response and Conclusions

Animation in the Macintosh environment has proven to be an effective medium for illustrating spatial concepts. We have shown the tutorial or selected modules to students at various stages in their undergraduate curriculum. They have found the tutorial highly user-friendly and have been impressed by the 3D color graphic display. All have appreciated the way it supplements the lecture experience and clarifies illustrations in their notes and texts. Although the tutorial is directed primarily at concepts important to understanding molecular structures of biological interest and for crystal lattices, its modules can be viewed independently as part of an introductory chemistry course or more advanced course in X-ray crystallography. It complements other teaching approaches, such as lectures, model building, and the use of Escher drawings (*16*).

Currently the tutorial is being expanded to include illustrations of higher symmetry point groups (tetrahedral, octahedral, icosahedral), glide planes, points of inversion, screw axes, and selected three-dimensional space groups. An archived copy of a current version of the program may be obtained by ftp. Please contact KAK (kant@fullerton.edu) to obtain access information.

# Spreadsheet-Controlled Potentiometric Analyses

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Spreadsheet programs running on microcomputers offer many advantages to scientists interested in an easy, user-friendly way of exploiting the power of the microcomputer without the time commitment usually required for learning a programming language. A spreadsheet's capabilities are especially valuable for problems involving repetitive calculations, graphics, large data sets, or those that involve What-If queries. A number of applications of spreadsheets in chemical education have been described, but only a few involve direct collection of experimental data into a spreadsheet (*17–21*).

## Direct Communication

A powerful feature of modern spreadsheets that is often overlooked is their ability to communicate directly with external devices through the computer's communication ports using the file commands available in a spreadsheet's macro programming language (*22*). A series of papers in *this Journal* described a number of such applications for the chemistry laboratory (*19–21*). In this report we describe two spreadsheet macro routines that complement this work, allowing direct control of a digital pH/mV meter through a serial interface. One program automates titration data collection, while the other automates data acquisition for potentiometric analyses that require the preparation of standard curves, such as ion-selective electrode analyses. The spreadsheet macros place the instrument's data directly into the appropriate spreadsheet cells. Because all instrument control and data acquisition are handled by the spreadsheet itself, there is no need to use programs in other languages to read data blocks into the spreadsheet, as in some previous work (*23–25*). The programs described here automate only the collection of the data and their placement in the worksheet, not the data reduction or plotting.

### *Titration Program*

In the titration program, the system is used to collect pH/mV data following the manual entry of buret readings at each step of a titration as titrant is added from a buret into the analyte solution. When the macro-containing worksheet is loaded, an autoexecuting routine displays a